

# Occam's Razor Cuts Away the Maximum Entropy Principle

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I show that the maximum entropy principle can be replaced by a more natural assumption, that there exists a phenomenological function of entropy consistent with the microscopic model. The requirement of existence provides then a unique construction of the related probability density. I conclude the letter with an axiomatic formulation of the notion of entropy, which is suitable for exploration of the non-equilibrium phenomena.

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The maximum entropy principle entered physics as a conclusion drawn by Gibbs from his description of classical statistical mechanics [1]. In its most proper form it was established by the theorem saying that: “*If an ensemble of systems is canonically distributed in phase, the average index of probability is less than in any other distribution of the ensemble having the same average energy*” [29]. Using a bit more modern language “the average index of probability” is the same as the average logarithm of the density, while the word “phase” simply refers to the phase space. I use the term “density”, in order to simultaneously cover both cases of a classical probability distribution and a quantum density operator. After Shannon had promoted the entropy to be the major quantity in information theory [2], the maximum entropy principle became, due to Jaynes, one of the fundamental laws of physics [3–5]. During the next more than 50 years this principle has found hundreds of applications in statistical mechanics (with emphasis on non-equilibrium phenomena) and information theory [6, 7]. With relatively little effort one can find examples from before the Jaynes formulation, in which the maximum entropy principle also played an important role in development of new theoretical concepts, such as relativistic thermodynamics [8].

It is probably a common feeling that the nature's tendency to maximize the entropy possesses a deeper philosophical meaning [9, 10]. While many scientists accept this tendency as being typical for physical theories, the unavoidable effort necessary to pick up the “maximal” scenario might raise some doubts (especially when it concerns the theory aiming at quantifying all kinds of efforts). The effort in question splits in fact into two subsequent tasks. First of all, we must exclude all cases which make the entropy depend on more average quantities (like the average energy) than anticipated. But this step we can as well make on the phenomenological level, by assuming that the entropy does depend only on the variables we are to use (or can experimentally access). There is no true necessity to invoke constrained optimization, to get rid of information we do not have anyway. It is enough to say that we fully rely on the

information which is accessible for us. The second task is the following: there exist many densities providing the entropy as a function of wanted parameters only, so it becomes necessary to select the maximal option.

So, is it eventually possible to avoid the requirement that the entropy must be maximal? The answer is yes, provided that the second problem listed above can be solved in a much simpler and physically more natural way. The aim of this letter is thus to prove that for a fixed, finite number of average parameters there is always *only* one density  $\varrho_0$  such that the entropy

$$-k_B \langle \ln \varrho \rangle_{\varrho}, \quad (1)$$

evaluated for  $\varrho = \varrho_0$  depends *only* (!) on these parameters, and the form of such *phenomenological entropy function*  $\mathcal{S}$  is preserved by all infinitesimal fluctuations of  $\varrho_0$ . According to a common notation  $\langle \cdot \rangle_{\varrho}$  denotes the average with respect to  $\varrho$ , while  $k_B$  is the Boltzmann constant but can as well be an arbitrary constant with a proper unit.

Before going into the details let me once more state the main message of this letter. Assume that we restrict ourselves to the phenomenological description based on a finite number of average parameters supplemented by the parameters which are constant (like the volume and the number of particles in the canonical ensemble). There exists the unique choice of the density (naturally the same as obtained by maximization [3, 4]) such that the entropy function depends only on the selected parameters and is microscopically given by the formula (1). The above statement happens to be too strong to be valid in general, since any family of densities involving a proper number of parameters can eventually be a good candidate for  $\varrho_0$ . But to make it true, it is sufficient to assume that whenever we infinitesimally change the density  $\varrho_0$  by  $\delta\varrho$ , the form of the phenomenological entropy  $\mathcal{S}$  remains the same, while the values of the involved average parameters change accordingly.

We can thus convert the maximum entropy principle to be the more plausible requirement of existence. As I show in the latter part, this remarkable property supports the microscopic definition of the entropy (1), because other

choices do not necessarily assure  $\varrho_0$  to be uniquely defined.

*The main result.*— Let me start the main discussion of this letter with few remarks about the notation. Considering a general landscape it becomes necessary to distinguish two sets of parameters. First of all we chose the variables  $\{\mathcal{V}\} = \{\mathcal{V}_1, \mathcal{V}_2 \dots\}$  which are assumed to be *externally fixed* (the number of these variables does not need to be specified). All variables relevant to the micro-canonical ensemble (energy, volume, number of particles) do belong to this set, while in the case of the canonical ensemble only the volume and the number of particles remain externally fixed. The second set of parameters is crucial for the Jaynes formulation of the maximum entropy principle [3, 4]. It consists of  $M$  additional variables ( $j = 1, \dots, M$ )

$$F_j \equiv F_j[\varrho_0], \quad (2)$$

represented by the linear functional  $F_j[\varrho] = \langle \tilde{F}_j \rangle_\varrho$  given in terms of the average values of some properly selected quantities  $\tilde{F}_j$ . In (i) the classical case,  $\tilde{F}_j$  are simply functions of the phase-space variables, while in (ii) the quantum case they are all Hermitian operators  $\hat{F}_j$ . We shall further distinguish the simplified case (ii-a) when all the operators commute with each other and the general case (ii-b) involving possibly non-commuting quantities.

Since the maximum entropy principle relies on constrained optimization, let me make a conceptual distinction. The naturally (always) present constraint on the norm of the distribution,  $\langle 1 \rangle_\varrho = 1$ , I shall call the *primary constraint*, while the additional constraints I shall call secondary. According to the maximum entropy principle, the density  $\varrho_0$  defining  $F_j$  is such that the entropy (1) becomes maximal, provided that the primary constraint and the secondary constraints (2) are satisfied. In this letter I shall provide an alternative derivation of the proper density  $\varrho_0$ .

While we do not plan to use the secondary constraints (2) directly, we cannot get rid of the primary constraint. We shall thus incorporate it into the analysis by defining the *microscopic entropy functional*

$$S_m[\varrho] = -k_B \langle \ln \varrho \rangle_\varrho - \lambda \left( \langle 1 \rangle_\varrho - 1 \right). \quad (3)$$

Since  $\lambda$  is an arbitrary parameter, the above formula strongly resembles the method of Lagrange multipliers. The term  $\lambda \left( \langle 1 \rangle_\varrho - 1 \right)$  is however here rather an artificial gauge which does not change the value of entropy, as long as the density  $\varrho$  is normalized. Even though Eq. (3) prepares the reader for an optimization routine and the next steps can bring more such similarities, I would strongly like to emphasize that the whole reasoning has nothing to do with any kind of optimization. All the formulas appearing below, being indeed very similar to those in the

method of the Lagrange multipliers, are purely functional identities.

Let me now assume that the phenomenological entropy

$$\mathcal{S} = \mathcal{S}(F_1, \dots, F_M; \{\mathcal{V}\}), \quad (4)$$

is a function of the parameters  $\{F\} = F_1, \dots, F_M$  and  $\{\mathcal{V}\}$ . Let me further introduce the corresponding *phenomenological entropy functional*

$$S_{\text{ph}}[\varrho] = \mathcal{S}(F_1[\varrho], \dots, F_M[\varrho]; \{\mathcal{V}\}). \quad (5)$$

By construction, we have that  $\mathcal{S} \equiv S_{\text{ph}}[\varrho_0]$ , so the macroscopic (phenomenological) entropy function  $\mathcal{S}$  is given by the functional (5) evaluated for  $\varrho = \varrho_0$ .

Note that the functionals  $S_m[\varrho]$  and  $S_{\text{ph}}[\varrho]$  are defined on the whole domain of  $\varrho$  and there are no secondary constraints spoiling this property. We can thus easily calculate the functional derivatives of both functionals:

$$\frac{\delta S_m[\varrho]}{\delta \varrho} = -k_B (1 + \ln \varrho) - \lambda, \quad (6)$$

$$\frac{\delta S_{\text{ph}}[\varrho]}{\delta \varrho} = \sum_{j=1}^M \left( \frac{\partial \mathcal{S}}{\partial F_j} \right)_{F_{k \neq j}} \frac{\delta F_j[\varrho]}{\delta \varrho}, \quad (7)$$

with the quantity  $\delta F_j[\varrho]/\delta \varrho$  being equal to  $\tilde{F}_j$ . The derivatives  $(\partial \mathcal{S}/\partial F_j)_{F_{k \neq j}}$  are  $\varrho$ -dependent functionals, and the thermodynamic notation  $(\cdot)_{F_{k \neq j}}$  has a usual meaning that we differentiate with respect to  $F_j$  keeping constant all other variables  $F_k$ , for  $k \neq j$ .

We are now ready to formally establish the main result of this letter. For a given set of parameters  $\{F\}$  and  $\{\mathcal{V}\}$ , there exist a unique density  $\varrho_0$  and a unique phenomenological entropy function  $\mathcal{S}$ , such that

$$S_m[\varrho_0 + \delta \varrho] - S_{\text{ph}}[\varrho_0 + \delta \varrho] = \mathcal{O}((\delta \varrho)^2), \quad (8)$$

or equivalently:

$$S_m[\varrho_0] = S_{\text{ph}}[\varrho_0] \equiv \mathcal{S}, \quad \left. \frac{\delta S_m[\varrho]}{\delta \varrho} \right|_{\varrho=\varrho_0} = \left. \frac{\delta S_{\text{ph}}[\varrho]}{\delta \varrho} \right|_{\varrho=\varrho_0}. \quad (9)$$

The physical meaning of the above conditions is straightforward. The left equation in (9) tells us that if  $\varrho = \varrho_0$ , the macroscopic entropy  $\mathcal{S}$  is not only given by the phenomenological entropy functional (what is true *per se*), but simultaneously originates from the microscopic model. It is however possible to find infinitely many couples of densities and entropy functions satisfying this matching requirement. The second, right condition is especially interesting. For a given couple  $(\varrho_0, \mathcal{S})$  fulfilling the left condition, we scan the infinitesimal neighborhood of  $\varrho_0$  and test if the form of the function  $\mathcal{S}$  is preserved. We expect that the true phenomenological entropy is attributed to the particular system treated as a whole, eg.

it captures the nature of the two-body interaction. On the other hand, possible infinitesimal fluctuations of the density, while enter the microscopic model, cannot affect the macroscopic character of the system in question (they cannot lead to a different global interaction mechanism). They could eventually change the values of the parameters describing the system, such as the average energy. From the physical perspective, this *stability* requirement is nothing more than a natural consequence of the fact, that the phenomenological entropy we have in mind, does really exist. Once more, let me emphasize that the conditions (9) say nothing about the optimization. They only give a mathematical meaning to our expectations, we have in relation to the macroscopic entropy  $\mathcal{S}$ .

Using the formulas (6, 7) we can solve the second equation from (9) with respect to  $\varrho_0$ , so that after taking into account the primary constraint we obtain the well-known expression for the density:

$$\varrho_0 = \frac{e^{-\sum_l \beta_l \tilde{F}_l}}{\langle 1 \rangle_{e^{-\sum_m \beta_m \tilde{F}_m}}}, \quad \beta_j = \frac{1}{k_B} \left( \frac{\partial \mathcal{S}}{\partial F_j} \right)_{F_{k \neq j}}. \quad (10)$$

The thermodynamic derivatives defining  $\beta_j$  are no longer functionals, but since  $\varrho = \varrho_0$  they become simple derivatives of the function (4). The density (10) is given by the exponential solution, similar in form to the solution provided by the constrained optimization. It is not incredibly surprising, because the exponential densities are known to be distinguished by the information-theoretic perspective [11], and are the unique distributions possessing a sufficient statistics [12]. The one and major difference is that in the optimization routine  $\beta_j$  are the Lagrange multipliers which must be found in such a way that the entropy becomes maximal. In our current case, these variables are the inverses of generalized temperatures (derivatives of the entropy).

It is not true that for any choice of the microscopic entropy functional, the  $\beta_j$  parameters would correspond to the derivatives of  $\mathcal{S}$ . However for (3) the above consistency requirement is satisfied, what seems to be a well-known fact in statistical mechanics [13]. Up to now, I have shown that the family of densities of the same form as given by the maximum entropy principle can be obtained without resorting to optimization. We could however expect, that in general it is possible to find many sets of parameters  $\beta_j$ , such that they are consistent with the secondary constraints (2) applied *a posteriori*. At that stage the crucial role of the maximum entropy principle would thus be to pick up the right set of  $\beta_j$ . But what if the last problem always possesses a unique solution? Then the maximum entropy principle can be completely eliminated in favour of the “phenomenologically motivated” condition of existence. The aim of the next paragraph is to prove that this scenario indeed occurs.

The secondary constraints (2) calculated for the expo-

ponential density (10) always provide the relation

$$F_j = f_j(\beta_1, \dots, \beta_M), \quad (11)$$

with  $f_j$  being some functions specific for the particular set of quantities  $\tilde{F}_j$ . If we assume that the number of average quantities  $M$  is finite, then the above formula in fact describes a map from  $\mathbb{R}^M$  to itself. In order to discuss the number of possible solutions to the system (16), we shall characterize the invertibility property of that map. This however means that we need to study its Jacobian matrix  $J_{ij} = \partial f_j / \partial \beta_i$ . In the cases (i) and (ii-a) we can easily find that the Jacobian matrix is:

$$J_{ij} = - \left( \langle \tilde{F}_i \tilde{F}_j \rangle_{\varrho_0} - \langle \tilde{F}_i \rangle_{\varrho_0} \langle \tilde{F}_j \rangle_{\varrho_0} \right). \quad (12)$$

The first term inside the parenthesis comes from the derivative of  $e^{-\sum_l \beta_l \tilde{F}_l}$ , while the norm  $\langle 1 \rangle_{e^{-\sum_m \beta_m \tilde{F}_m}}$  is responsible for the second one. The Jacobian matrix is equal to minus the covariance matrix evaluated for the set of quantities  $\tilde{F}_j$ . We thus obtain a very important conclusion: if the quantities  $\tilde{F}_j$  are chosen in such a way that they are *linearly independent*, then their covariance matrix is positive-definite, and the map (16) is everywhere locally invertible. But if instead of all the variables  $F_j$  we consider  $-F_j$ , then the Jacobian matrix of the corresponding map sending  $(\beta_1, \dots, \beta_M)$  to  $(-F_1, \dots, -F_M)$  will be positive-definite as well. This however turns out to be the sufficient condition for a global invertibility of the map [14, 15] so that there always exists a unique solution  $\beta_l = (f^{-1})_l(-F_1, \dots, -F_M)$ .

The case (ii-b) is much more technical, because in order to evaluate the derivatives of  $e^{-\sum_l \beta_l \tilde{F}_l}$  we need to use the operator formula [16]

$$\partial_\eta e^{-\hat{A}(\eta)} = - \int_0^1 dz e^{(z-1)\hat{A}(\eta)} \frac{\partial \hat{A}(\eta)}{\partial \eta} e^{-z\hat{A}(\eta)}. \quad (13)$$

It turns out [13, 17], that the Jacobian matrix is equal to  $J_{ij} = -2 \int_0^{1/2} dz \text{CM}(z)$ , and involves the symmetrized covariance matrix [18]  $\text{CM}(z) =$

$$\frac{1}{2} \left\langle \hat{F}_i(z) \hat{F}_j^\dagger(z) + \text{h.c.} \right\rangle_{\varrho_0} - \langle \hat{F}_i(z) \rangle_{\varrho_0} \langle \hat{F}_j(z) \rangle_{\varrho_0}, \quad (14)$$

evaluated for the set of *dressed*, non-Hermitian operators  $\hat{F}_i(z) = e^{-z\hat{R}} \tilde{F}_i e^{z\hat{R}}$ , with  $\hat{R} = -\frac{1}{2} \sum_l \beta_l \tilde{F}_l$ . In fact, only the first term of the above covariance matrix depends on  $z$ , because the operators  $e^{\pm z\hat{R}}$  cancel each other under the average of a single dressed operator. A much more important observation is however that the procedure of dressing does not change the mutual relations between the operators. As long as  $\tilde{F}_i$  are chosen independently, their counterparts  $\hat{F}_i(z)$  are also linearly independent. Since for every value of  $z$  the symmetric covariance matrix  $\text{CM}(z)$  must be positive-definite [19], this property is inherited by  $-J_{ij}$ . We can immediately apply the previous reasoning to complete the whole proof.

*Discussion.*— The most important conclusion from the above considerations is the fact that we can formulate a new axiomatic definition of the notion of entropy. It reads: *there exists a unique choice of the entropy function  $\mathcal{S}$  such that: (1) on the phenomenological level  $\mathcal{S} \equiv \mathcal{S}(\{F\}; \{\mathcal{V}\})$  depends only on a given collection of externally fixed variables  $\{\mathcal{V}\}$  and a finite number  $M$  of average values  $F_j \equiv F_j[\varrho_0]$ , (2) on the microscopic level  $\mathcal{S} \equiv \mathcal{S}[\varrho_0]$  is given by the formula  $\mathcal{S}[\varrho] = -k_B \langle \ln \varrho \rangle_{\varrho}$  evaluated for  $\varrho = \varrho_0$ , (3) the stability condition  $\mathcal{S}[\varrho_0 + \delta\varrho] = \mathcal{S}(\{F\}; \{\mathcal{V}\}) + \epsilon$  with  $F_j = F_j[\varrho_0 + \delta\varrho]$  and  $\epsilon = \mathcal{O}((\delta\varrho)^2)$  is valid for any infinitesimal variation  $\delta\varrho$ .* Moreover, the associated density  $\varrho_0$  belongs to the exponential family.

The axiomatic formulation leads to several conclusions relevant for the theory of statistical mechanics. First of all, the notion of the microcanonical ensemble as well as the postulate of equal a priori probability follow immediately. It is sufficient to set  $M = 0$ , so that because  $\mathcal{S}$  cannot depend on average values, the exponential form of  $\varrho_0$  boils down to the constant value. This value is determined by the energy  $E$ , the volume  $V$  and the number of particles  $N$  which are all the externally fixed variables. The canonical ensemble appears if we set  $M = 1$  and take  $\hat{F}_1$  to be the Hamiltonian. The exact form of the Hamiltonian (as long as mathematically reasonable) does not affect the validity of this simple picture.

Further analysis of the axiomatic definition of entropy brings a new understanding to notions, such as a generalized (when we consider more averages than the energy) quasi-static thermodynamic transformation, or a non-equilibrium state. The first concept is described by a situation when during the time evolution the phenomenological entropy depends on the fixed set of parameters, and only the values of the particular parameters can change. A signature of non-equilibrium appears immediately when the description based on a certain number  $M$  becomes physically insufficient, so that we need to increase  $M$ , or the third axiom is no longer satisfied. From a mathematical point of view, an interesting question is under which conditions the operation of changing the number of relevant thermodynamical variables can be done in a continuous, or even smooth, manner. That could happen by letting the parameters  $\beta_j$  related to the new quantities to grow in time, being identically equal to 0 in the past. Finally, an interesting perspective would be to understand if the case  $M = \infty$  is a typical scenario appearing in non-equilibrium statistical mechanics, and if the answer is yes, to understand how efficiently the system could be described in terms of a finite number of phenomenologically distinguished parameters. An adventurous challenge would be to design a kind of  $\varrho$ -dependent measure of complexity, able to capture the relevant value of  $M$ .

Another recently developing conceptual challenge,

namely the attempts to establish a joined theory of quantum information and quantum thermodynamics [20–22], could as well benefit from the philosophical nature of the observation that there is no necessity to maximize the entropy. In fact, this observation remains valid when other kinds of accessible information given in terms of non-sharp inequality constraints on the probability distribution are taken into account. They do not affect the derivation presented in this letter, but only restrict the domain of the global variables used.

Finally, the maximum entropy principle has been extensively used as a tool to develop new facets of statistical mechanics based on microscopic entropies different than (1), eg. (Rényi or Tsallis) [23–28]. An important issue would be to examine these results in the context of the present letter. The uniqueness property seems to distinguish the logarithmic form of entropy, the other entropy functionals are thus indeed expected to go beyond the usual way of reasoning. They might as well turn out to be unique, provided that additional conditions (axioms) are satisfied.

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## Appendix

The density operator in the case (ii-b) is given by:

$$\varrho_0 = \Lambda^{-1} \exp \left( - \sum_l \beta_l \hat{F}_l \right), \quad \Lambda = \text{Tr} \exp \left( - \sum_l \beta_l \hat{F}_l \right), \quad (15)$$

so that Eq. (11) explicitly reads:

$$F_j = f_j(\beta_1, \dots, \beta_M) = \Lambda^{-1} \text{Tr} \left[ \hat{F}_j \exp \left( - \sum_l \beta_l \hat{F}_l \right) \right]. \quad (16)$$

With the help of the general formula (13) providing the parameter-derivative of the exponent of a parameter-dependent operator we find:

$$J_{ij} = \frac{\partial f_j}{\partial \beta_i} = - \left( \text{Tr} \left( \hat{F}_j \hat{G}_i \right) - \text{Tr} \left( \hat{F}_j \varrho_0 \right) \text{Tr} \hat{G}_i \right), \quad (17)$$

where

$$\hat{G}_i = \Lambda^{-1} \int_0^1 dz e^{2(1-z)\hat{R}} \hat{F}_i e^{2z\hat{R}}. \quad (18)$$

First of all, we observe that since the trace is invariant under cyclic permutations, we easily get:

$$\begin{aligned}\text{Tr} \hat{G}_i &= \Lambda^{-1} \int_0^1 dz \text{Tr} \left( e^{2(1-z)\hat{R}} \hat{F}_i e^{2z\hat{R}} \right) \\ &= \int_0^1 dz \text{Tr} \left( \hat{F}_i \varrho_0 \right) \\ &= \text{Tr} \left( \hat{F}_i \varrho_0 \right).\end{aligned}\quad (19)$$

In the second step, we shall split the integration range in (18) into two intervals  $[0, 1/2]$  and  $[1/2, 1]$ , and in the second interval perform the change of variables  $z \mapsto 1 - z$  to get:

$$\hat{G}_i = \Lambda^{-1} \int_0^{1/2} dz \left( e^{2(1-z)\hat{R}} \hat{F}_i e^{2z\hat{R}} + e^{2z\hat{R}} \hat{F}_i e^{2(1-z)\hat{R}} \right). \quad (20)$$

The above formula in terms of the  $\hat{F}_i(z)$  operators read:

$$\hat{G}_i = \int_0^{1/2} dz \left( e^{-z\hat{R}} \varrho_0 \hat{F}_i(z) e^{z\hat{R}} + \text{h.c.} \right). \quad (21)$$

Using once more the invariance of the trace we thus obtain

$$\text{Tr} \left( \hat{F}_j \hat{G}_i \right) = \int_0^{1/2} dz \text{Tr} \left( \hat{F}_i(z) \hat{F}_j^\dagger(z) \varrho_0 + \text{h.c.} \right). \quad (22)$$

Since the term  $\text{Tr} \left( \hat{F}_j \varrho_0 \right) \text{Tr} \hat{G}_i$  does not depend on  $z$ , it can be “multiplied” by  $2 \int_0^{1/2} dz$ . On the other hand, the average values of the dressed operators are the same as those for the undressed ones, i.e.

$$\text{Tr} \left( \hat{F}_j \varrho_0 \right) = \text{Tr} \left( \hat{F}_j(z) \varrho_0 \right) = \text{Tr} \left( \hat{F}_j^\dagger(z) \varrho_0 \right). \quad (23)$$

All the above observations boil down to the desired formula [Eq. (14) and the expression for  $J_{ij}$  appearing above it] with the average  $\langle \cdot \rangle_{\varrho_0}$  understood in terms of the trace  $\text{Tr}(\cdot \varrho_0)$ .

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